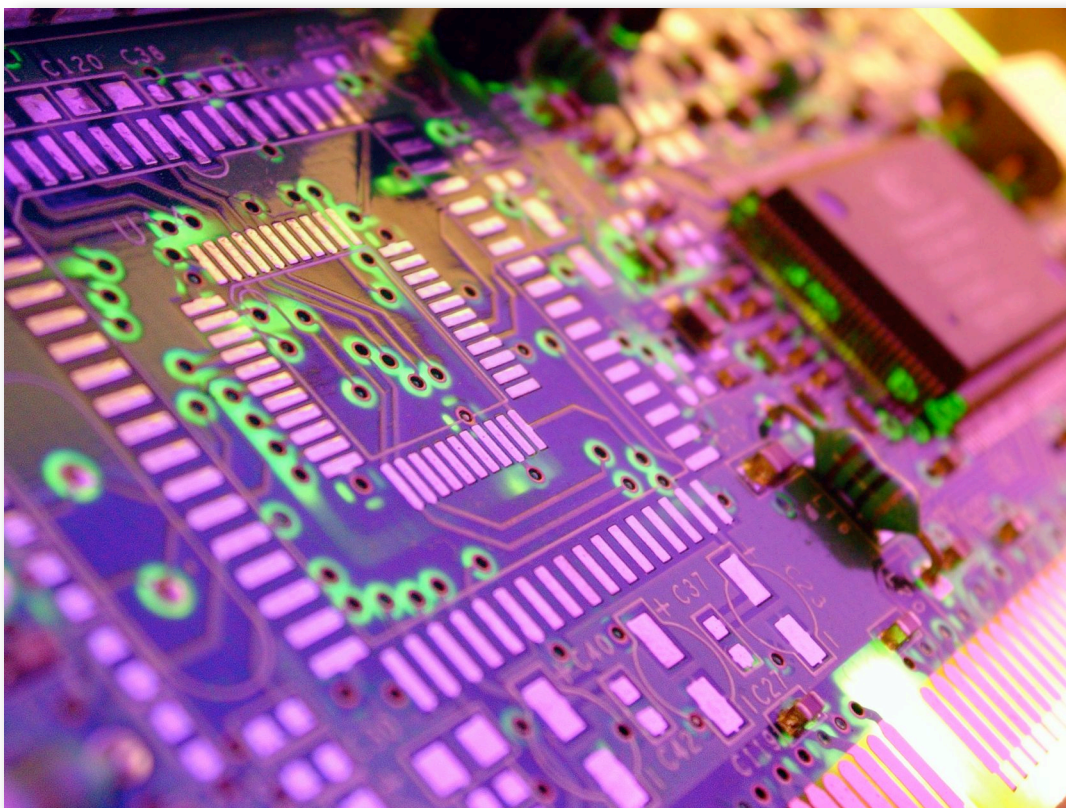


ELECTRICAL CIRCUIT & DEVICE CAPABILITIES



UNIQUE CAPABILITIES DESIGNED TO SUPPORT SANDIA

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Introduction

Electrical Modeling & Simulation Overview

Group 1430, Computational Sciences R&D, specializes in the development of innovative modeling and simulation tools and solutions for Sandia customers in the areas of electrical circuit, devices and microsystems. Our modern software applications and world-class research offer unique and leading-edge numerical and computational resources that enable physical understanding for discovery, design and analysis.

Production-level applications include the Xyce™ Parallel Electronic Simulator and the Charon semiconductor device simulator. These tools, designed to run easily on single workstations or massively parallel computers and clusters, currently support customers in Stockpile Life Extension Programs, Integrated Stockpile Evaluation, and the Qualification Alternatives to the Sandia Pulse Reactor (QASPR) project, as well as other key missions of Sandia. Our goal is to help bring Center 1400's world-class R&D capabilities in all aspects of high-performance computing to maturity in production-level tools in support of the larger Laboratories missions. In addition to these tools abilities' to harness the computational power of large-scale computers, they also provide other differentiating capabilities such as advanced solver algorithms and radiation-aware models.

Our work in developing codes for high performance simulation of electrical devices and circuits is complemented by our theory and modeling research on the underlying materials physics issues. We have simulation capabilities and expertise in semiconductor physics, with particular emphasis on the effects of radiation-induced damage on performance and electrical breakdown in dielectrics. Radiation effects are characterized using theory and a hierarchical multiscale computational approach. Results from quantum calculations are combined with a continuum theory calculation of radiation-induced defects in oxides and semiconductors to provide accurate PDE-based descriptions of relevant defect physics mechanisms for use in both Xyce and Charon.

Our Products

Production-level software tools in the Center span several levels of fidelity including device-scale semiconductor modeling (with radiation effects) using the Charon code. Charon is a modern, fully parallel device simulation code employing state-of-the-art discretization and solutions methods to advance capabilities in device-scale modeling. Its development is currently being driven largely by the demands of QASPR, Sandia's effort to help offset the loss of fast-transient neutron testing facilities with modeling and simulation combined with enduring testing capabilities. In supporting this mission, Charon is also developing the world's most advanced radiation-aware device performance and defect modeling capabilities internal to its physics formulation. Additionally, and most importantly, when complete, these capabilities will also be rigorously verified and validated to ensure accurate solutions of problems where margins are a critical driver.



One step further up the abstraction hierarchy is the Xyce circuit (analog) modeling code, also with radiation effects models. Due to its parallel scalability, the Xyce code is regularly used to model digital circuits at the analog (transistor) level to evaluate performance of these large integrated circuits. Questions



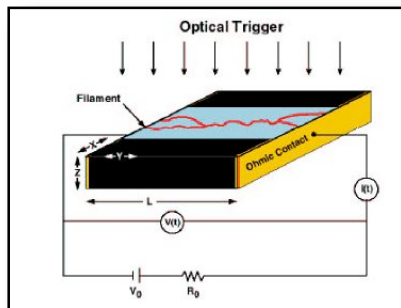
answered at this scale that cannot be answered using traditional digital (timing) models include power consumption and radiation effects on performance and power. Additionally, Xyce may be coupled to digital simulators to perform mixed-signal analysis. This capability is currently in a prototype stage but expected

to be delivered as a production capability in a future release.

Both of these products have been designed from the ground-up as scalable parallel applications. However, they run equally well on single processor or small-scale parallel workstations and support a variety of operating systems. See their specific sections below for a more complete list of supported computing hardware.

Our R&D Capabilities

Two additional software tools support the development of the physics models electrical device behavior that is incorporated into Charon and Xyce. These are REOS, a 2-D research code that solves the drift-diffusion equations and is used to evaluate the macroscopic electrical response of candidate defect reaction mechanisms, and QUEST, an efficient code that applies the Density Functional Theory (DFT) for computing the quantum behavior of a material. REOS is used to test theoretical ideas of the physical processes governing electrical device response, especially under unusual operating conditions. QUEST is used to characterize defects in semiconductors and oxides, identify reaction mechanisms and then quantify the reaction rates. This information greatly helps in determining values for the physical parameters occurring in the continuum description simulated in both REOS and Charon.



Another example of our theory and modeling research is developing an explanation of the light-initiated conductivity discovered by Sandia researchers and now being applied in the photoconductive semiconductor switch as a sprytron replacement. This work resulted in a general theory of electrical breakdown in solids. Testing of this theory is on-going.

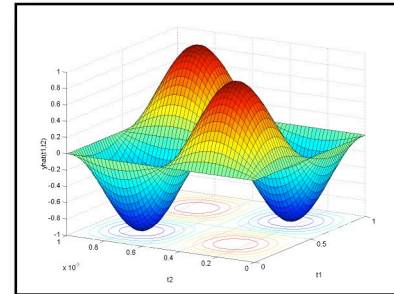
Integration

Within Group 1430, the staff understand and value the contributions each code and research project area make towards realizing the end capability of simulating electrical circuit behavior with emphasis on the unique requirements of Sandia's missions. The managers of the two key departments (1435 and 1437) encourage these interactions and actively support the team to extend and apply high performance computing modeling and simulation capability to Sandia mission problems.

Circuit Modeling - Xyce

The Xyce Parallel Electronic Simulator provides improved circuit simulation capability over other available tools in the following differentiating areas:

- **Size** - Capability to solve extremely large circuit problems at the transistor level by supporting large-scale parallel computing platforms (up to thousands of processors). Note that this also includes support for most popular parallel and serial computers.
- **Speed & Robustness** - Improved performance for all numerical kernels (e.g., time integrator, linear solver) through utilization of Sandia's world-leading algorithms and solver libraries (<http://software.sandia.gov/Trilinos>) as well as novel techniques designed specific for Sandia's circuit modeling community.
- **Flexibility** - Support for modeling circuit phenomena at a variety of abstraction levels (device, analog, digital and mixed-signal) in a rigorous and tightly coupled manner, allowing for timely, full-system solutions.
- **Applicability** - Radiation-aware (x-ray, gamma and neutron) as well as aging device models. Additionally, most of Sandia's MDL technologies are supported (e.g., CMOS-6 and CMOS-7 with ViArray coming soon).
- **Portability** - A client-server or multi-tiered operating model, wherein the numerical kernel can operate distinct from the simulation interface (Xyce is part of the ESimTools project; please see <http://sass2152.csu891.sandia.gov/esimtools> for more information). Xyce also runs on most desktop systems including MS Windows (2000 and XP), Apple OS X, and Red Hat Linux.
- **Maintainability** - Object-oriented code design and implementation using modern coding practices that ensure that the Xyce Parallel Electronic Simulator will be maintainable and extensible far into the future.
- **Accuracy** - Rigorously verified and validated code and device-model implementations for regimes of interest to Sandia customers. This distinction is critical where design margins are tight and environments are extreme.



Xyce is a parallel code in the most general sense of the phrase – a message passing parallel implementation – which allows it to run efficiently on the widest possible number of computing platforms. These include serial, shared-memory and distributed-memory parallel platforms. Furthermore, careful attention has been paid to the specific nature of circuit simulation problems to ensure that optimal parallel efficiency is achieved even as the number of processors grows.

As mentioned above, the Xyce Parallel Electronic Simulator has been developed in support of the unique requirements of electrical designers and analysts at Sandia and, as those needs continue to evolve, Xyce will adapt to continue aligning with those needs.

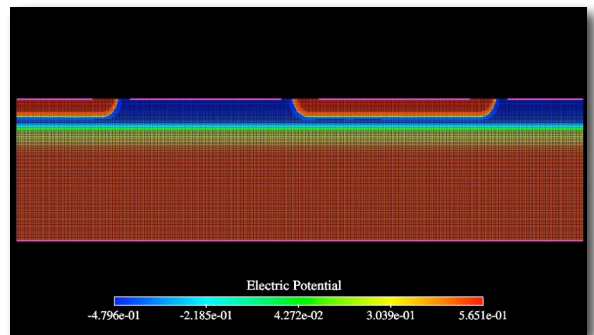
For more information on Xyce, please visit <http://www.cs.sandia.gov/xyce/> for the Sandia external site or <http://sass2152.csu891.sandia.gov/esimtools/xyce.html> for the Sandia internal site.

Device Modeling - Charon

The Charon project seeks to model electrical semiconductor devices (e.g., transistors) at high fidelities using the drift-diffusion equations. By applying finite element and massively parallel solver technology developed at Sandia, this tool will be capable of modeling semiconductor device behavior at unprecedented fidelity including transient gamma and neutron irradiation effects. Relying on the Nevada finite element framework and the Trilinos solver toolkit (both leading-edge Sandia software products), rapid development of robust and scalable capability has been achieved. The Charon tool is critical to the Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) effort allowing computational modeling to assist in the qualification of weapons systems under high radiation environments.

Key areas of capability beyond current commercial tools include:

- **Size** - Capability to solve extremely high fidelity semiconductor device problems including support for radiation effects due to the massively parallel, distributed memory capability. Existing commercial codes are typically limited to simulating problems with less than 10^6 elements while Charon will support problems with up to 10^8 elements.
- **Robustness & Accuracy** – Application of stabilized finite element techniques and advanced numerical algorithms allow unprecedented robustness and accuracy of solution.
- **Applicability** – User control of radiation defect physics allows the analyst to easily research candidate mechanisms and the sensitivity of a device to such mechanisms.



Model Research & Development

Radiation: X-Ray & Gamma

One of the unique features of the Xyce circuit simulator is its ability to simulate radiation effects in transistor devices. Initial efforts, in collaboration with 1700, have focused on modeling X-Ray and Gamma effects, or photocurrent effects. Photocurrent is caused by a large amount of energy being deposited in semiconductor material, which results in a very high ionization rate. The large number of electron-hole pairs, created through ionization, will contribute to currents far outside normal device operation in the presence of an electric field. These conditions are met near PN junctions. The models that have been implemented in Xyce are generally a superset of legacy transistor models, with additional physics-based nonlinear equations added to model these photocurrent effects.

Radiation: Neutron

Neutron effects are also of interest, but are much less well understood than photocurrent. While a qualitative understanding of neutron effects has existed since the 1960's, it has been insufficient to create models that are physics-based and predictive. Qualitatively, neutron bombardment results in damage to the semiconductor crystalline lattice, which results in increased energy levels in the band structure. The additional energy levels are often recombination centers, and can cause significant gain degradation in the devices. Over time, the device will recover through annealing. Empirical models of this effect exist, but the development of more scientific understanding is one of the objectives of the QASPR project (see below). Ultimately, this improved understanding will result in physics-based neutron models in Xyce. Charon and QUEST are actively being used to help develop this understanding.

Aging: ELDRS

Radiation effects tests in the late 1990's revealed that, for a given total radiation dose, silicon devices exhibited an increased sensitivity to damage when the radiation is applied at a lower rate. This phenomenon became known as the Enhanced Low Dose-Rate Sensitivity. From several years of theoretical and computational investigation, supported by Advanced Simulation and Computing (ASC) and the Enhanced Surveillance Campaign (ESC), H. Hjalmarson (1435) succeeded in explaining ELDRS as the result of the action of several different bimolecular reactions occurring in the oxide layer and at the oxide-silicon interface that involve hydrogen, protons, electrons, and holes. Each reaction mechanism leads to a reduced radiation effect at high dose rates. This research led to a physics-based model that can be used to assess the low-dose rate aging of silicon microelectronics in the stockpile to aid Sandia's surveillance efforts.

Current Projects & Customers

QASPR

In response to a directive from NNSA requiring Sandia to shut down its pulsed reactor, SPR III, which is used for qualification of electrical components and subsystems to hostile environments, in FY05 Sandia launched the Qualification Alternatives for the Sandia Pulse Reactor (QASPR) project. The goal of QASPR is to develop a process for qualifying weapon electronics using enduring testing capabilities combined with high performance modeling and simulation. The suite of simulation codes currently envisioned for this process is illustrated in Figure 1. The simulation process begins by calculating, with the NuGET code, the neutron and gamma fluxes impinging on warhead electronics. The Cascade code is then used to determine the types and concentrations of lattice defects created from collision of a high energy neutron with a silicon atom. When greater accuracy is needed in simulating the end of the damage cascade that results from the recoil of the initial silicon atom, a high fidelity molecular dynamics calculation is performed with the GRASP code. The defect type and concentration information is then used in DFT calculations with QUEST to characterize defect energies and properties, and these also serve as inputs to the Charon device simulations. QUEST calculation results are also used in REOS to test ideas of defect evolution and develop the defect reaction descriptions (constitutive models) required by Charon to simulate the evolving device performance. Charon and Xyce will be used in conjunction to perform the detailed device and circuit response simulations that will be needed for the qualification process.

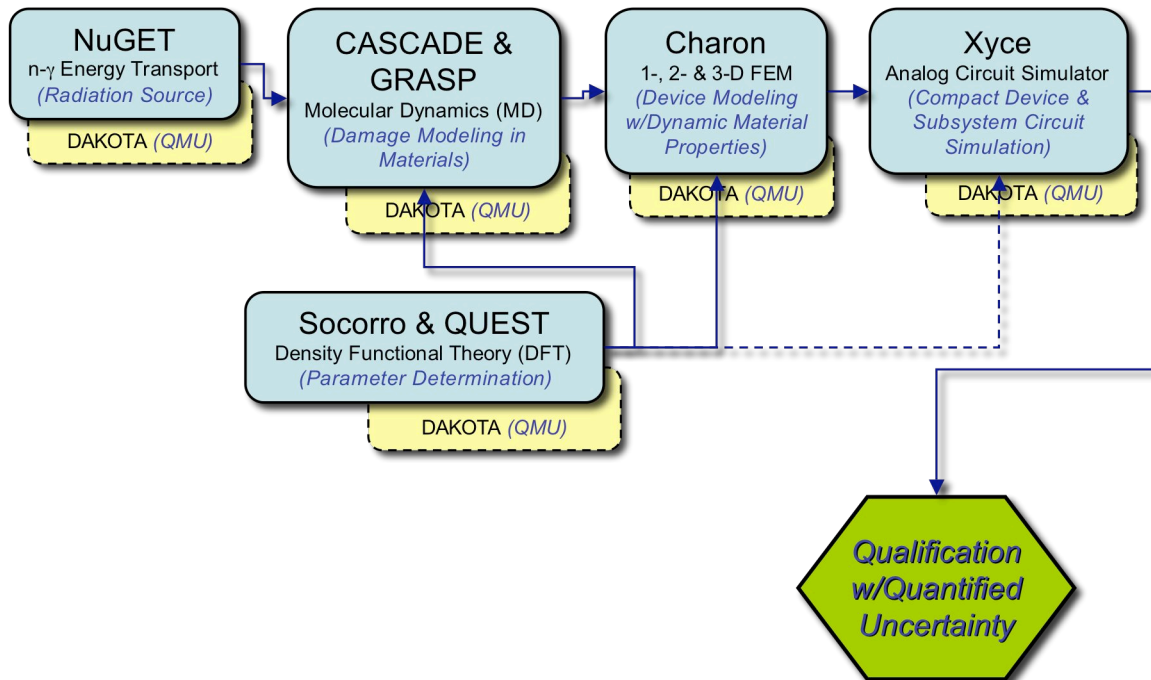


Figure 1. QASPR M&S Code Integration



Group 1430 developed and owns the majority of the modeling and simulation codes currently involved in the QASPR project. These codes include QUEST (Density Functional Theory - DFT), GRASP (Molecular Dynamics - MD), Charon (device modeling) and Xyce (circuit modeling). Additionally, the REOS code (device modeling) is also being used to support model development and discovery as Charon continues to be developed. When QASPR began in FY05, Group 1430 already had these capabilities in either development or in a state of production so that these tools were the obvious choice for the project. Since then, the staff in 1430 have strengthened their working relationship within the Group and developed strategic ones with the staff and management involved with the broader QASPR project.

W76-1 AFS

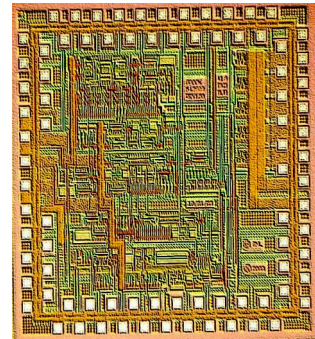
The Xyce team in 1437 is working with a team of electrical analysts in 8205 who are performing circuit calculations to help strengthen the technical basis for qualification of the W76-1 AFS to radiation environments. In particular, the teams are working closely with designers in 5350 to construct and simulate circuit models of the Driver and Logic Assembly boards within the AFS including the Permafrost 2 (PA2) ASIC that uses Sandia's radiation hard CMOS7 process. These models include appropriate radiation-aware devices that will be used to model performance under hostile conditions. Also part of this project is a validation effort for the various device models and the larger assembly model that will provide uncertainty, margins and confidence information associated with the simulation results. The results of these efforts are expected to be used as part of the Technical Basis for the W76-1 qualification and will be presented to the Navy in the Producibility Design Review in FY06.

Enhanced Surveillance

The Xyce team is also working with staff in Departments 12346 (Weapons Surety Engineering) to bring its circuit modeling and simulation capabilities to bear on problems involving the enduring stockpile. In particular, Xyce is being used to characterize and bound aging effects on stockpile electronics as part of the Model Based Performance Analysis (MBPA) project. This project provides modeling and simulation support to the Component Surveillance Program (CSP) by identifying key devices to focus research and testing. Additionally, it provides a predictive capability to the Enhanced Surveillance Campaign (ESC) by identifying trends in device characteristics because of aging and the impact upon system performance margins.

Microelectronics Development Laboratory

Since the release of Xyce 1.0, a cooperative relationship has developed between the Xyce developers and designers in 1700. One such example was the simulation of the W80-3 SA3989 (A.K.A. Spock) Firing-Set Application Specific Integrated Circuit (ASIC). The ASIC is a mixed-signal multi-function DC-to-DC power supply controller chip and is comprised of approximately 4500 transistors fabricated in the MDL CMOS6R radiation hardened process. Xyce was used to simulate the function of this ASIC when a commercial simulator not only failed to run the necessary simulation to completion but also produced erroneous results for the portion it completed.



Xyce has been used to simulate a variety of digital and mixed-signal ASICs produced by the MDL including the Permafrost-2 (PA2) as mentioned above.

Summary

Group 1430 has made strategic investments and partnered throughout Sandia to help provide unique and leading-edge research and tools to support electrical modeling and simulation. These capabilities are designed with Sandia's needs in mind and leverage research into high-performance computing and scalable solution algorithms, additional strengths within Center 1400. The experienced staff anticipates new and exciting applications of their work to problems at Sandia and their management team looks forward to helping continue to impact Sandia customers in the area of electrical modeling and simulation.

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